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Math & Scientific Libraries

MKL

DRAFT

This article is being reviewed for completeness and technical accuracy.

The Intel Math Kernel Library (MKL) is composed of highly optimized mathematical functions for engineering and scientific applications requiring high performance on Intel platforms. The functional areas of the library include linear algebra consisting of LAPACK and BLAS, fast Fourier transform (FFT), and vector transcendental functions.

MKL release 10.x is part of the Intel compiler 11.0 and 11.1 releases. Once you load in a 11.x compiler module, the path to the MKL library is automatically included in your default path. If you choose to use Intel compiler 10.x or earlier versions, you have to load an MKL module separately.

A Layered Model for MKL

Starting with MKL release 10.0, Intel employs a layered model for the MKL library. The layers are:

- Interface layer
    - ♦ LP64 interface (uses 32-bit integer type) or ILP64 interface (uses 64-bit integer type)
    - ♦ SP2DP interface

      which supports Cray-style naming in applications targeted for the Intel 64 or IA-64 architecture and using the ILP64 interface. SP2DP interface provides a mapping between single-precision names (for both real and complex types) in the application and double-precision names in Intel MKL BLAS and LAPACK.
- Threading layer
    - ♦ sequential

      The sequential (non-threaded) mode requires no Compatibility OpenMP* or Legacy OpenMP* run-time library, and does not respond to the environment variable OMP_NUM_THREADS or its Intel MKL equivalents. In this mode, Intel MKL runs unthreaded code. However, it is thread-safe, which means that you can use it in a parallel region from your own OpenMP code. You should use the library in the sequential mode only if you have a particular reason not to use Intel MKL threading. The sequential mode may be helpful when using Intel MKL with programs threaded with some non-Intel compilers or in other situations where you may, for various reasons, need a non-threaded version of the library (for instance, in some MPI cases).

Note that the *sequential.* library depends on the POSIX threads library (pthread), which is used to make the Intel MKL software thread-safe and should be listed on the link line.

- threaded

  The *threaded* library in MKL version 10.x supports the implementation of OpenMP that many compilers (Intel, PGI, GNU) provide.

- Computational layer

  For any given processor architecture (IA-32, IA-64, or Intel(R) 64) and OS, this layer has only one computational library to link with, regardless of the Interface and Threading layer.

- Compiler Support Run-time libraries

  - libiomp

    Intel(R) Compatibility OpenMP run-time library

  - libguide

    Intel(R) Legacy OpenMP run-time library

For example, to do a dynamic linking of myprog.f and parallel Intel MKL supporting LP64 interface, use:

```
ifort myprog.f -Wl,--start-group -lmkl_intel_lp64 \
-lmkl_intel_thread -lmkl_core -Wl,--end-group -openmp
```

If you are unsure of what MKL libraries to link with, use the suggestion provided in this Intel web site by providing the proper OS (e.g. Linux), processor architecture (e.g. Intel(R) 64), compiler (e.g. Intel or Intel Compatible), dynamic or static linking, integer length, sequential or multi-threaded, OpenMP library, cluster library (e.g. BLACS, ScaLAPACK), MPI library (Intel MPI, MPICH2, SGIMPT, etc.).

The -mkl Switch of Intel Compiler Version 11.1

Starting from Intel compiler version 11.1, a -mkl switch is provided to link to certain parts of the MKL library.

```
-mkl[=]
          link to the Intel(R) Math Kernel Library (Intel(R) MKL) and
          bring in the associated headers
            parallel   - link using the threaded Intel(R) MKL libraries.
                         This is the default when -mkl is specified
            sequential - link using the non-threaded Intel(R) MKL libraries
            cluster    - link using the Intel(R) MKL Cluster libraries plus
                         the sequential Intel(R) MKL libraries
```

The libraries that are linked in for

```
    * -mkl=parallel

          --start-group \
          -lmkl_solver_lp64 \
          -lmkl_intel_lp64 \
          -lmkl_intel_thread \
          -lmkl_core \
          -liomp5 \
          --end-group \

    * -mkl=sequential

          --start-group \
          -lmkl_solver_lp64_sequential \
          -lmkl_intel_lp64 \
          -lmkl_sequential \
          -lmkl_core \
          --end-group \

    * -mkl=cluster

          --start-group \
          -lmkl_solver_lp64 \
          -lmkl_intel_lp64 \
          -lmkl_cdft_core \
          -lmkl_scalapack_lp64 \
          -lmkl_blacs_lp64 \
          -lmkl_sequential \
          -lmkl_core \
          -liomp5 \
          --end-group \
```

Where to find more information about MKL

Man pages and two PDF files from Intel are available for each version of MKL.

- Man pages of Intel MKL

  A collection of man pages of Intel MKL functions are available under the man3 subdirectory (e.g., /nasa/intel/Compiler/11.1/072/man/en_US/man3) of the MKL installation. You will have to load an MKL module or an Intel compiler 11.x module before you can see the man pages. For example,

```
% module load comp-intel/11.1.072
% man gemm
```

provides information about [s,d,c,z,sc,dz]gemm routines.

Unfortunately, there does not appear to be a 'man mkl' page.

- Intel MKL Reference Manual (mklman.pdf)

  Contains detailed descriptions of the functions and interfaces for all library domains:

  - BLAS
  - LAPACK
  - ScaLAPACK
  - Sparse Solver
  - Interval Linear Solvers
  - Vector Math Library (VML)
  - Vector Statistical Library (VSL)
  - Conventional DFTs and Cluster DFTs
  - Partial Differential Equations support
  - Optimization Solvers

- Intel MKL User's Guide (userguide.pdf)

  Provides Intel MKL usage information in greater detail:

  - getting started information
  - application compiling and linking depending on a particular platform and function domain
  - building custom DLLs
  - configuring the development environment
  - coding mixed-language calls
  - threading
  - memory management
  - ways to obtain best performance

The two pdf files can be found in the 'doc' or 'Documentation' directory of the MKL installation. For example, on Pleiades,

- MKL version 10.0.011

  /nasa/intel/mkl/10.0.011/doc

- The version included in the Intel compiler module 11.1.072

  /nasa/intel/Compiler/11.1/072/Documentation/en_US/mkl

SCSL

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SCSL is a comprehensive collection of scientific and mathematical functions that have been optimized for use on the Altix systems such as Columbia . The libraries include optimization of basic linear algebra subprograms (BLAS), a linear algebra package, signal processing functions such as fast Fourier transforms (FFTs), and liner filtering operations and other basic solver functions. More information can be found through 'man scsl'.

```
Starting with ProPack 5, SCSL is no longer supported by SGI.
Although SCSL is still available on Columbia (but not on Pleiades),
users are recommended to use Intel MKL instead.
```

SCSL version(s) available on Columbia systems:

- scsl.1.5.0.0 (does not work properly with intel-comp.9.1.039)
- scsl.1.5.1.0
- scsl.1.5.1.1 (contains Scalapack in libsdsm.so)
- scsl.1.6.1.0

To use SCSL, link one of the following libraries:

```
-lscs
-lscs_mp      (for multi-threaded programs)
-lscs_i8
-lscs_i8_mp
```

MKL FFTW Interface

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Some users have installed the FFTW library in their own directory (for example, /u/user/bin/fftw) and would link to the FFTW library as follows:

```
ifort -O3
  -I/u/user/bin/fftw/include   \
  -o fftw_xmpl.exe fftw_xmpl.f \
  -L/u/user/bin/fftw/lib -lfftw3
```

An MKL FFTW interface has been created for Intel compiler version 11.0.083 and later versions. Users no longer have to keep their own copy of FFTW. Follow these steps to use the MKL FFTW interface:

- Load a compiler module 11.0.083 or a later version such as comp-intel/11.1.072

  ```
  module load comp-intel/11.1.072
  ```

- Compile and link

  ```
  ifort -O3                                             \
    -I/nasa/intel/Compiler/11.1/072/mkl/include/fftw    \
    -o fftw_xmpl.exe fftw_xmpl.f                        \
    -lfftw3xf_intel -lmkl_intel_lp64 -lmkl_intel_thread \
    -lmkl_core -lguide
  ```